

# Informatics for Materials Science and Basic Chemicals Research

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#### Joint Project with Accenture- 2002

- define mat/chem informatics needs
- Scope- global chemicals synthesis R&D group
  - Includes all their high-throughput work.
  - Includes leveraged organizations.

#### Goals

- Preliminary requirements gathering
- Preliminary architecture (technical, product, systems)
- Implementation proposal
  - with cost estimate



#### What did we find?

- We do synthesis research in, e.g.,:
  - Michigan, Texas, West Virginia, Switzerland, California
- Seems we've bought at least 1 of everything...

We want all the data available to everyone.



#### The things you learn...



- People want to see all the data...
  - But they don't want to enter it themselves.
- People want to know what others have done...
  - But use their own vocabulary and work practices.
- People know the reactor makes a difference...
  - But they haven't named their reactors.



#### Discovery vs. Process Research

- Discovery Research
  - Screening
  - Yes/No or ID tests
  - Looking for an event
  - # samples large
  - # condition sets small

- Process Research
  - Optimization
  - Mixture analysis
  - Measurement precision
  - # samples small
  - # condition sets large
  - Data integration
    - With other reactors
    - Across scales



#### **Key Components of our Architecture**

- Experimental design
- Experiment control
- Data collection
- Result management
- Supporting data mgmt.
- ETL

- Sample/entity tracking
- Materials inventory
- Compound registry
- Data model
- Data visualization
- Diagnostics



#### **Key Informatics Operational Components**

**Network stability** 

IT systems support

User support

Diagnostics



# The Lesson of **Process Analytical Chemistry**

Q: How do you know when the analyzer breaks?

A: Diagnostics



#### Is Dow

a Big Enough Chemical Company

to Afford Informatics?



#### A Tale of Two Economies

Profit as a % of Sales

Pharmaceuticals 15-20%

Chemistry 3-4%

R&D Spending as a % of Sales

Pharmaceuticals 15-20%

Chemistry3-4%

Source- 2001 Fortune 500 list



#### The Following is

a Biased Perspective

**Based on Too Little Knowledge** 



#### A Successful Business Model in Pharmaceuticals

Find, develop and sell the next "blockbuster" drug.

Keep the price high while patented.

Use profits to fund your next discovery.



# Does This Model Work for Materials and Basic Chemicals?

NO!



#### What's Different?

- Materials & Basic Chemicals are commodities.
- The money isn't there to pay big R&D costs.

• There is no "prescription materials" insurance.



#### Can We Afford the High-Tech Solution?





#### The Story of Halsey Pharmaceuticals- No Bull!

During the last several years, Halsey has sought to diversify its businesses through strategic acquisitions and alliances and through the development and manufacture of APIs used by others as raw materials in the manufacture of finished pharmaceutical forms. In this regard, the Company has acquired exclusive licenses and also internally developed novel synthesis technologies that the Company expects to develop and use in the manufacture of APIs intended for use in a broad range of ... products.



#### Does this Business Model Sound Familiar?

- How's it working?
  - Total sales 2002
    - \$7.8MM
  - R&D spending
    - \$1.6M (20%)
  - Business results
    - (\$4.9MM)



#### **TEVA Pharmaceuticals**

World's largest generic drug maker

- 2002 sales- \$2.5B

- 2002 R&D spending- \$165MM (6.6%)\*

- 2002 EBIT- \$499MM (20%)

\* Mostly for new active discovery/development



#### More Comparisons to Pharma

- We have many more "targets".
- Our measurement technology is...
  - more complex.
  - less standardized.
- Our taxonomy is...
  - See above



#### **How Do We Change the Game?**

- Take a lesson from Pharma
  - Generics- effective, cost less
- Software
  - Buy vs. build
- Taxonomy, inter-operability, communication
  - Develop and adopt standards

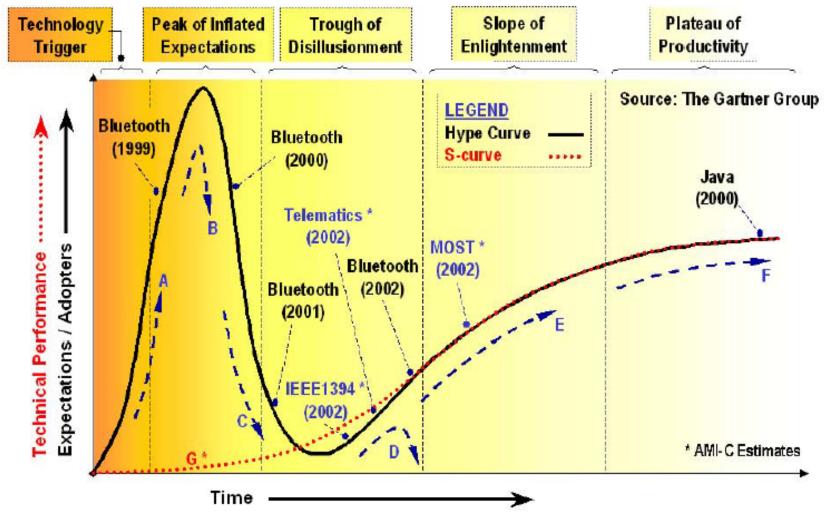


#### The Late-Adopter Benefit

- Early adopters pay the big bills
  - Code development
  - Discovering product shortcomings
  - Discovering requirements
  - Developing standards



#### Stages of the Hype Cycle





#### Challenge to the Industry

- Continue to press for standards in all phases of technology development
- Work on synchronized application releases for enabling technologies



### **More Challenges**

- Enabling, non-competitive technologies must be interoperable; find ways to work together
- Bring a multi-technology, seamless communication system to automotive

Ken Khangura, Chief Engineer,
Fast Cycle Products, Ford Motor Company
TelematicsUpdate Seminar, Las Vegas,
January 8, 2003



## Go "Forth" and Multiply



"No man can serve two masters: for either he will hate the one, and love the other; or else he will hold to the one, and despise the other."

Matthew 6:24



#### Materials and Basic Chemistry R&D

We were the #1 customers for analytical technology in the 60's and 70's.

Not any more.

Somebody is and we'd better align with them...



#### **Conclusions**

## The challenges are:

Culture change

Affordability

Standardization